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ESTIMATING THE UNCERTAINTY AND PREDICTIVE CAPABILITIES OF THREE-DIMENSIONAL EARTH MODELS (POSTPRINT)

Annual Report 3

Delaine T. Reiter, et al.

Weston Geophysical Corporation
181 Bedford St., Suite 1
Lexington, MA 02420

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AIR FORCE RESEARCH LABORATORY
Space Vehicles Directorate
3550 Aberdeen Ave SE
AIR FORCE MATERIEL COMMAND
KIRTLAND AIR FORCE BASE, NM 87117-5776

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Delaine T. Reiter[1], William L. Rodi[2], and Stephen C. Myers[3]

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181 Bedford St., Suite 1
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Weston Geophysical Corporation[1], Massachusetts Institute of Technology[2], and Lawrence Livermore National Laboratory[3]

14. ABSTRACT

A maximum likelihood approach to solving the geostatistical estimation problem is being pursued whereby the geostatistical parameters, together with pick-error variances, are simultaneously fit to the second-order statistics of the observed travel-time residuals. The maximum likelihood criterion for the optimal parameter values reduces to a set of coupled, nonlinear equations which, in general, must be solved numerically. The geostatistical estimation problem within a maximum-likelihood framework has been formulated and an approach for its numerical solution outlined.

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ESTIMATING THE UNCERTAINTY AND PREDICTIVE CAPABILITIES OF THREE-DIMENSIONAL EARTH MODELS

Delaine T. Reiter[1], William L. Rodi[2], and Stephen C. Myers[3]

Weston Geophysical Corp.[1], Massachusetts Institute of Technology[2], and Lawrence Livermore National Laboratory[3]

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ABSTRACT

In recent years many models of three-dimensional (3-D) seismic velocity structure in Eurasia have been developed using a variety of techniques and data. Most of these models are not accompanied by quantitative estimates of uncertainty, either in the model parameters themselves (e.g. seismic velocities) or in geophysical observables predicted by the models (e.g. body-wave travel times). Moreover, the various 3-D models produced by these studies have not been compared to one another in their predictive capabilities in any meaningful way within the monitoring research community. To address these issues we are developing and applying evaluation metrics that robustly quantify and compare the uncertainty and predictive capability of 3-D seismic velocity models.

There are two major elements in our approach. First, we are performing a comprehensive evaluation of a set of 3-D velocity models for Eurasia based on previously developed data misfit and event mislocation metrics. These metrics are computed using a ground-truth (GT) data set available at the International Seismic Centre (ISC). We discuss some of the progress we have made in reconciling discrepancies between the parameterization and coverage of various models available to the research community, and compare some of the standard metrics we have been able to derive for these models.

Second, we are investigating a new approach to evaluating velocity models based on a Bayesian framework for model uncertainty in the travel-time tomography problem. In this approach, geostatistical parameters describing velocity heterogeneity in the Earth are estimated from travel-time residuals observed along a set of event-station paths. The parameters include the velocity variance, which quantifies the strength of velocity heterogeneity, and vertical and horizontal correlation lengths, which quantify the spatial smoothness of velocity heterogeneity. The inferred geostatistical parameters characterize the discrepancy between the Earth's velocity and the velocity of the reference model used to calculate the travel-time residuals. That is, they quantify the uncertainty of the reference model and thus serve as metrics for model evaluation. In addition, as we have shown in previous projects, geostatistical parameters can be used to calculate the uncertainty in travel times predicted by the reference model for arbitrary paths. We formulate the geostatistical estimation problem within a maximum-likelihood framework and outline an approach for its numerical solution.

We are currently pursuing a maximum likelihood approach to solving the geostatistical estimation problem whereby the geostatistical parameters, together with pick-error variances, are simultaneously fit to the second-order statistics of the observed travel-time residuals. The maximum likelihood criterion for the optimal parameter values reduces to a set of coupled, nonlinear equations which, in general, must be solved numerically. We formulate the geostatistical estimation problem within a maximum-likelihood framework and outline an approach for its numerical solution.

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OBJECTIVES

The main objective of our project is to develop meaningful measures of the predictive capabilities of the multitude of models that have been developed over recent years by the nuclear monitoring research community. While our primary focus is on regional-scale seismic velocity models, we intend our general approach to be applicable as well to global Earth models and models of other geophysical parameters such as attenuation and density.

Our project consists of two major elements. First, we have collected a set of regional 3-D velocity models for Asia and are performing a comprehensive and methodical evaluation of them using data misfit and event mislocation metrics. Metrics will be evaluated for each model based on a common ground-truth data set comprising GT5 events and their arrival picks. A large part of this effort so far has been spent developing standardized methods for model parameterization, forward modeling (e.g. ray tracing), and event relocation. Some of the tools we need for these tests are available to us in-house from our previous tomography and location projects, but others are being gathered from outside sources.

The second element of our project is the investigation of a new approach for estimating the uncertainty and predictive capability of 3D velocity models. Our approach will quantify model uncertainty in terms of spatially variable geostatistical parameters fit to second-order statistics of travel-time residuals, and then convert these parameters into the uncertainty in travel-time or other geophysical predictions. To do this requires covariance modeling capabilities we developed for travel times in an earlier project (Rodi and Myers, 2008) and which can be extended to other observables.

RESEARCH ACCOMPLISHED

3-D Seismic Velocity Models, Ground-Truth Data, and Analysis Techniques to Examine Model Performance

Our first task has been to collect 3-D regionalized seismic velocity models and format them in a way that makes comparisons straightforward. Table 1 lists the six velocity models that we are currently using in our study, along with their respective authors and a brief description. Our test-bed model for the project is the Joint Weston/MIT (JWM) inversion model (Reiter and Rodi, 2009). JWM is the result of a joint inversion of regional P travel times and Rayleigh fundamental-mode group velocities. It consists of the P and S velocities and density of the crust and upper mantle for a broad region of Asia (defined in a geographic box from 10 – 50°N, 40 – 110°E). In addition to the JWM model, we have obtained the CUB2.0 surface-wave inversion model (Ritzwoller et al., 2002) with density; the Stevens et al. (2008) surface-wave inversion model; the EAV09 inversion model from the group headed by Suzan van der Lee at Northwestern University (Schmid et al., 2008); and a new P-velocity inversion model (LLNL_G3-D) from Nathan Simmons and Stephen Myers (Simmons et al., 2011). We also have access to an *a priori* regionalized model known as the DOE Unified Model (Begnaud et al., 2004; Pasyanos et al., 2004). We continue to seek models from other researchers, but many are not openly available or do not meet the necessary criteria to be included in our study.

One of the more difficult problems we have encountered in the project has been the difficulty in accurately representing the models in our study using a single common format. At the present time there is no standardized format for model exchange, which has prevented the community and program funding managers from understanding the significant differences between 3-D models that are constructed for use in predicting nuclear monitoring observables. Our in-house model format represents a 3-D model as a geographic grid of 1-D profiles, with each profile sharing a common parameterization with respect to depth. For example, in the JWM model the crust at each latitude/longitude point is divided into vertically homogeneous layers corresponding to the those of the CRUST2.0 model: water overlying two sediment layers (soft and hard sediments) overlying three metamorphic/igneous layers (upper, middle and lower crust). The upper mantle is represented vertically by piecewise linear parameter functions sampled at multiple nodes distributed between the Moho discontinuity and a depth of 410 km. The versatility of this model format allows discontinuities and homogeneous layers to be accurately captured, and no special software is necessary to allow the models to be exchanged between researchers. Most of the models in our study can be represented in this format, although some conversion is necessary in certain cases (LP2008; Stevens et al., 2008).

We believe that the seismic monitoring community would be well served by developing and adopting a standard Earth model exchange format. Other research communities have long-standing efforts in this area. For example, the international climate modeling community developed a standard protocol in 1990 for global atmospheric general circulation models (AGCMs) that provides a framework in support of climate model diagnosis, validation,

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intercomparison, documentation and data access. Their framework enables a diverse community of scientists to analyze AGCMs in a systematic fashion, which serves to facilitate model improvement (Gates, 1992). Our research community would also benefit greatly from the development of a framework for model exchange, similar to the one the seismic community has for data exchange.

Table 1. Descriptions of the current set of 3-D seismic velocity models used in the study.

Model Name	Authors	Geographic Coverage	Type	References
JWM	Weston/MIT	10 - 50°N, 30 - 120° E	*inversion* model of Vp, Vs and density; constructed with Pn travel times and Rayleigh group velocities	Reiter and Rodi (2009)
LLNL G3D	LLNL	Global, high-res over MidEast	*inversion* model of Vp constructed from P and Pn travel times	Myers *et al.* (2011); Simmons *et al*. (2011)
DOE Unified Model	LLNL/LANL	0 - 85°N, 20 - 75° E	*a priori* model of Vp, Vs, density, Qp and Qs	Pasyanos *et al*., 2004; Begnaud *et al*., 2004
CUB20_J362D28	CU Boulder Harvard	Global	*inversion* model of Vp, Vs and density from 0 - 700 km defined over the globe; determined with group velocities	Shapiro and Ritzwoller, 2002
LP2008	SAIC	Global	*inversion* model of Vp, Vs, density, Qbeta from 0 - ~700 km defined over the globe; determined with surface waves	Stevens *et al*., 2008
EAV09	Northwestern Univ./ LLNL	10 - 60°N, ~35 - 80° E	*inversion* model of Vs with add'l conversion to Vp; determined mainly from waveforms and teleseismic S travel times	Schmid *et al*., 2008

To demonstrate the usefulness of performing simple model comparisons, Figure 1 displays map-view slices from the models in our study. The geographic coverage of the maps in Figure 1 was chosen based on the footprint of the JWM model, which means that two of the models do not completely cover their respective plots (LLNL_G3D is global, but we only requested a certain piece of it, and the EAV09 model is concentrated on the Middle East). The Generic Mapping Tool (GMT) package (Wessel and Smith, 1995) was used to plot the P and S velocities at a depth of 90 km, using the same color map for each model. Prior to creating this plot, the models were reformatted to our in-house 3-D parameterization and then interpolated to a depth-slice grid. The different panels in Figure 1 offer a direct comparison of the models and illustrate their similarities and differences. For example, JWM, LLNL_G3D and CUB2.0 are similar to each other in the strength of heterogeneities at this upper-mantle depth. All models demonstrate similar patterns of slow- and fast-velocity areas across the plotted region. CUB2.0 is defined on a 2°x2° grid, which produces a smoother result compared to the other models. The EAV09 model is similar to other models in its shear velocity values, but the P velocities appear to exhibit weaker overall variation compared to the other models. The LP2008 model is 'blocky' in nature, which is to be expected since it is comprised of homogeneous layers that are conducive to dispersion modeling calculations. The *a priori* LLNL Unified model is least like the others in pattern and heterogeneity strength – we note that this model is equivalent to the 3SMAC model (Nataf and Ricard, 1996) at this depth.

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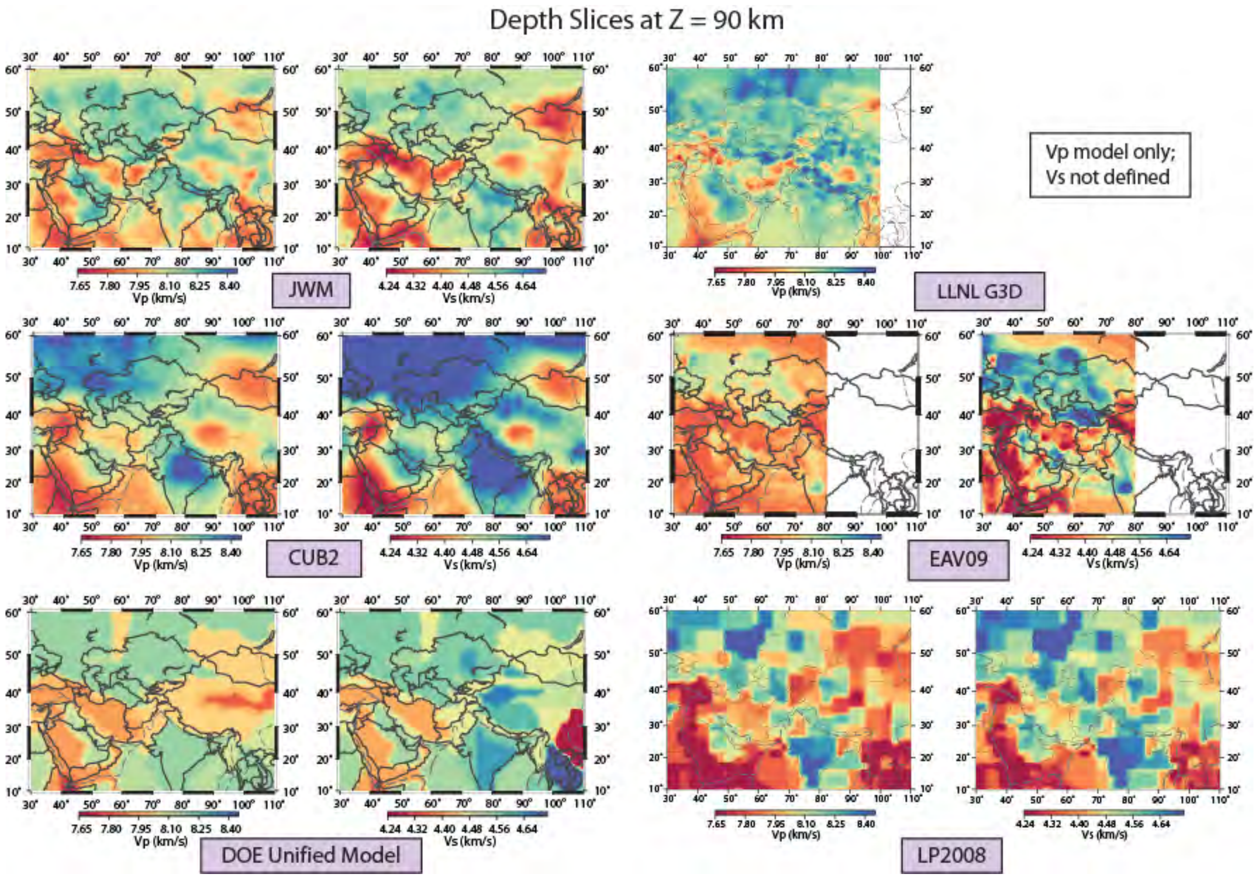

Figure 1. Map-view slices of P and S velocity at 90 km depth from the regional 3-D velocity models in our study (see Table 1). The models are labeled at the bottom of each Vp and Vs plot, and the color scale is the same across all panels. See the text for further explanation of these plots.

To evaluate models with respect to one another, we require a high-quality set of GT events whose epicentral locations are known precisely. We used the new catalog of GT0-5 reference events (Bondár and McLaughlin, 2009) hosted by the ISC (http://www.isc.ac.uk). This global database includes more than 7,000 events whose epicentral location accuracy is known to at least 5 km. GT events with well-established locations and origin times have been used by multiple authors to validate velocity models (Ritzwoller et al., 2003; Flanagan et al., 2007). We filtered the new International Association of Seismology and Physics of the Earth's Interior (IASPEI) Reference Event List (REL) for events in our study region and found 248 GT0–5 explosions and 348 GT5 earthquakes, most of which are in specific geographic clusters. From these events we extracted the defining regional P and S arrival-time picks in the IASPEI REL that were used to develop the GT locations.

Using a variety of filtering criteria designed to eliminate outliers, we derived a validation data set of 9,242 P-wave and 2,214 S-wave regional arrivals observed at stations within a latitude-longitude box defined by (0-60° N, 30-120° E). The great-circle raypath coverage for the P and S GT observations is shown in Figure 2. While the S GT observations are not strictly needed for most of the model validation exercises that we perform, we included them with the idea they may be useful in future studies. It is clear that the current version of our GT data ray paths sample only a limited portion of the JWM study region, which illustrates the difficulty of validating a model with travel times alone. However, the IASPEI REL database is currently the highest quality GT data resource we have to demonstrate the performance of the 3-D models.

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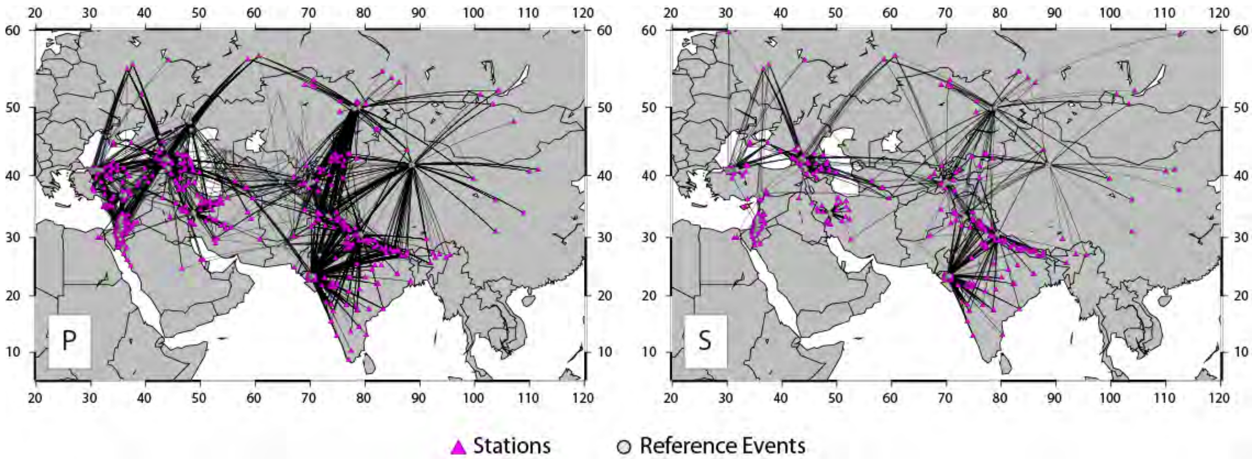

Figure 2. Great-circle raypath coverage for the P (left) and S (right) paths in the IASPEI REL ground-truth database. Stations are represented by purple triangles and events by gray circles. Note the sparse coverage over the area of the regional 3-D models.

We have begun to augment the GT0-5 IASPEI REL data set with other observations that have been collected in previous research efforts. While these supplemental databases may only be of GT10-20 quality in the event locations, they can still provide insights into the travel-time prediction behavior of the various models, and they are a valuable data source for testing the variance estimation approach we are pursuing under the second major task of the project. For instance, a consortium effort led by SAIC in the early 2000s produced several valuable GT data resources that are not included in the IASPEL REL (Murphy et al., 2005). The electronic supplement that accompanies the Murphy et al. (2005) paper contains several groomed event bulletins that we plan to utilize in our study. One of these is specifically focused on China and consists of travel-time observations at 49 stations of the dense Chinese National Network that were used in a tomographic inversion. Murphy et al. (2005) notes that the average quality of the Chinese bulletin locations is on the order of GT10, making them suitable for use in a broad number of validation studies. Figure 3 shows the distribution of stations and events in the Chinese tomographic inversion bulletin that we have begun to analyze for use in metric performance calculations.

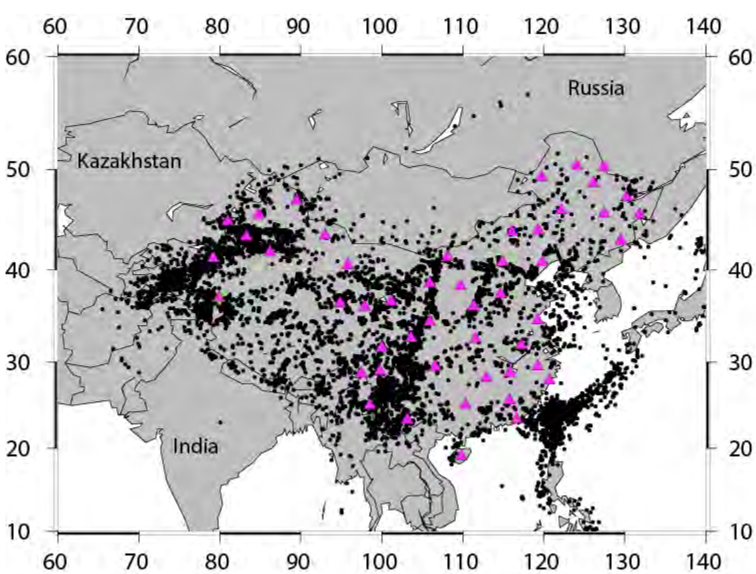

Figure 3. Supplemental ground-truth data set from the Chinese ABCE bulletin, collected under a previous nuclear monitoring research consortium effort (Murphy et al., 2005). The events are shown as black dots, and the Chinese stations as purple triangles.

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While Figure 1 illustrates that the 3-D models in our study can seem quite different in snapshot form, they often perform like each other in travel-time prediction and location tests. To examine these behaviors we are investigating the performance of the 3-D models using different forward modeling techniques, in an attempt to determine whether, how and why they differ. For example, in Figure 4 we show the results of predicting the ray path from a GT0 explosion in the Western Soviet Union to station SHI in Iran, using all six models in Table 1 and the Podvin-Lecomte (1991) ray tracing method. The epicentral path length for the event-station pair is approximately 13.6° and in the IASPEL REL the bulletin observation is 194 s for the travel time of the Pn phase. The station-path map is shown in the center of Figure 4, and arrayed around the map are summed projections (collapsed to Cartesian latitude) of the ray paths that each 3-D model produces for the station-event pair that we chose. In each inset ray path sub-panel we list the bottoming point of the ray and the travel time along the path.

The results show that three of the models produce ray paths that meet a classical definition of the Pn phase, traveling near the base of the Moho discontinuity in the uppermost mantle. However, three of the models produce ray paths that dive deeper into the mantle along a traditional P-wave trajectory, bottoming at depths greater than 140 km. The path travel times also vary fairly significantly across the six models, with a spread of ~7 seconds. It is interesting to note that all of the models have Moho depths close to 45 km on both the station and event sides of the ray paths, so further analysis is warranted to explain the wide variation in the ray path behaviors for this case.

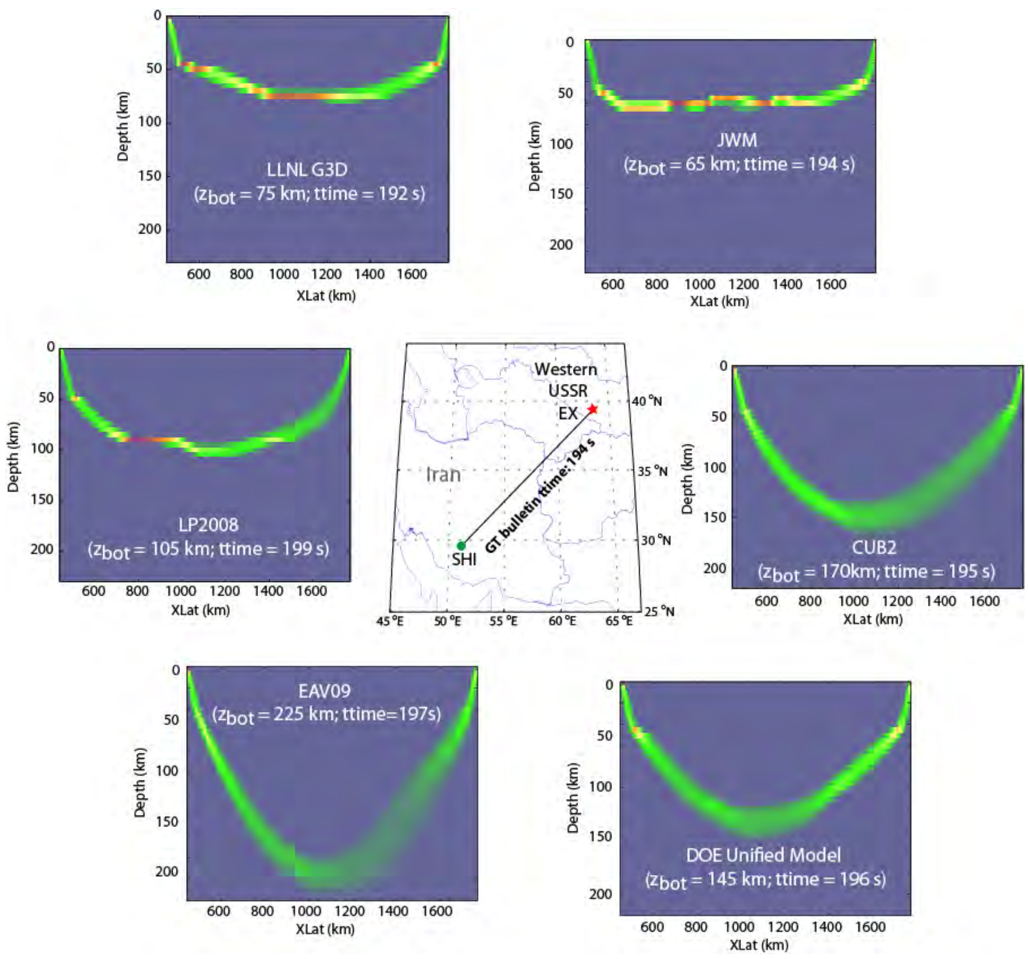

Figure 4. Example illustrating the ray path behavior in each 3-D model for a single event-to-station pair in the ground-truth database. The rays are comprised of the sensitivities calculated along the particular path by the Podvin-Lecomte method; they are depicted as projections (summations) to latitude.

The results of this type of exercise illustrate the significant differences that can exist in the subsurface spatial sampling and travel times of a given ray path across the various models. We are analyzing the differences between

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different ray tracing techniques (e.g. ray-bending, ray shooting, fast marching method, eikonal) to see how the model performance changes. Our aim is to determine whether the prediction/forward modeling techniques used to *develop* individual 3-D Earth models must be included as part of the distribution of a new model within the research community.

Evaluation of Velocity Models Based on Model Uncertainty Analysis

To address the second major task in our project, we have developed a mathematical framework for the problem of estimating geostatistical parameters of velocity heterogeneity in the Earth from travel-time residuals observed along a set of event-station paths. The inferred geostatistical parameters characterize the discrepancy between the Earth's velocity and the velocity of the reference model used to calculate the travel-time residuals. That is, they quantify the uncertainty of the reference model and thus serve as metrics for model validation. In addition, as we have shown in previous projects, geostatistical parameters can be used to calculate the uncertainty in travel times predicted by the reference model for arbitrary paths.

The problem can be formulated mathematically as follows. Let the vector $\mathbf{m}$ contain parameters describing the difference between the slowness functions of the real Earth and a reference model. Then a vector of observed travel-time residuals $\mathbf{r}$, calculated with respect to the reference model, can be related to $\mathbf{m}$ to first order by

$$\mathbf{r} = \mathbf{Am} + \mathbf{e}, \tag{1}$$

where $\mathbf{A}$ is a travel-time sensitivity matrix and $\mathbf{e}$ is a vector containing measurement (pick) errors in the residuals. The pick errors are assumed to be zero mean with some variance/covariance matrix $\mathbf{C}_e$. Likewise, we assume $\mathbf{m}$ is zero mean with variance $\mathbf{C}_m$. Equation 1 then implies that $\mathbf{r}$ is zero mean with variance matrix given by

$$\mathrm{E}[\mathbf{r}\mathbf{r}^T] \equiv \mathbf{C}_r = \mathbf{A}\mathbf{C}_m\mathbf{A}^T + \mathbf{C}_e. \tag{2}$$

Now assume that $\mathbf{C}_e$ is a given function of a parameter vector $\underline{\theta} = (\theta_1\,\theta_2\,\cdots)^T$, and that $\mathbf{C}_m$ is parameterized by $\underline{\gamma} = (\gamma_1\,\gamma_2\,\cdots)^T$. The θ_k, for example, might be pick-error variances as a function of epicentral distance. The γ_k are the geostatistical parameters of interest, comprising slowness variances and correlation lengths as a function of position in the Earth. The problem at hand is to infer the parameters θ_k and γ_k from $\mathbf{r}$ on the basis of Equation 1, recognizing that the γ_k are the primary targets.

We have examined a number of possible approaches to solving this variance estimation problem and are currently pursuing a formal approach based on maximum-likelihood estimation. The relevant likelihood function is provided by the probability density function of $\mathbf{r}$. Assuming $\mathbf{m}$ and $\mathbf{e}$, and thus $\mathbf{r}$, are Gaussian, the likelihood function, L, is given by

$$\log L\left(\underline{\theta}, \underline{\gamma}\right) = const - \tfrac{1}{2}[\log(\det \mathbf{C}_r) + \mathbf{r}^T\mathbf{C}_r^{-1}\mathbf{r}], \tag{3}$$

where it is understood that $\mathbf{C}_r$ depends on $\underline{\theta}$ and $\underline{\gamma}$. The optimal estimates of these parameter vectors are the values that maximize L. This implies that L is stationary with respect to the parameters, or

$$\frac{\partial L}{\partial \theta_k} = 0, \quad \frac{\partial L}{\partial \gamma_k} = 0. \tag{4}$$

Given Equations 2 and 3, and the properties of matrix determinants, the stationarity conditions become

$$\mathrm{trace}\; \mathbf{C}_r^{-1}\frac{\partial \mathbf{C}_e}{\partial \theta_k} = \mathbf{r}^T\mathbf{C}_r^{-1}\frac{\partial \mathbf{C}_e}{\partial \theta_k}\mathbf{C}_r^{-1}\mathbf{r} \tag{5}$$

$$\mathrm{trace}\; \mathbf{C}_r^{-1}\mathbf{A}\frac{\partial \mathbf{C}_m}{\partial \gamma_k}\mathbf{A}^T = \mathbf{r}^T\mathbf{C}_r^{-1}\mathbf{A}\frac{\partial \mathbf{C}_m}{\partial \gamma_k}\mathbf{A}^T\mathbf{C}_r^{-1}\mathbf{r}. \tag{6}$$

These equations can be simplified by substituting the theoretical results of tomographic inversion implied by the stochastic assumptions we have made. That is, the maximum *a posteriori* (MAP) estimate of $\mathbf{m}$, and its residual vector, are given by

$$\tilde{\mathbf{m}} = \mathbf{C}_m\mathbf{A}^T\mathbf{C}_r^{-1}\mathbf{r} \tag{7}$$

$$\tilde{\mathbf{e}} = \mathbf{r} - \mathbf{A}\tilde{\mathbf{m}} = \mathbf{C}_e\mathbf{C}_r^{-1}\mathbf{r}. \tag{8}$$

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Also useful are the influence and resolution matrices, **S** and **R**, respectively:

$$\mathbf{S} = \mathbf{A}\mathbf{C}_m\mathbf{A}^T\mathbf{C}_r^{-1} \tag{9}$$

$$\mathbf{R} = \mathbf{C}_m\mathbf{A}^T\mathbf{C}_r^{-1}\mathbf{A}. \tag{10}$$

Equations 5 and 6 can then be rewritten as

$$\text{trace } (\mathbf{I} - \mathbf{S})\frac{\partial \mathbf{C}_e}{\partial \theta_k}\mathbf{C}_e^{-1} = \tilde{\mathbf{e}}^T\mathbf{C}_e^{-1}\frac{\partial \mathbf{C}_e}{\partial \theta_k}\mathbf{C}_e^{-1}\tilde{\mathbf{e}} \tag{11}$$

$$\text{trace } \mathbf{R}\frac{\partial \mathbf{C}_m}{\partial \gamma_k}\mathbf{C}_m^{-1} = \widetilde{\mathbf{m}}^T\mathbf{C}_m^{-1}\frac{\partial \mathbf{C}_m}{\partial \gamma_k}\mathbf{C}_m^{-1}\widetilde{\mathbf{m}}. \tag{12}$$

Equations 11 and 12 are coupled, nonlinear equations that cannot be solved analytically except in very simple situations. In a problem involving a large number of residuals and slowness parameters, efficient numerical solution schemes are also elusive. The difficulty of the problem depends on the particular choice of the parameters θ_k and γ_k. We are in the process of devising iterative, numerical algorithms for solving Equations 11 and 12 for pick-error and slowness variances, holding correlation lengths of slowness heterogeneity fixed. If the resulting algorithms are efficient, the solution for correlation lengths can possibly be found by grid search or trial-and-error, if more direct schemes are not discovered.

CONCLUSIONS AND RECOMMENDATIONS

The main objective of our research project is to develop and apply meaningful measures of the predictive capabilities of 3-D Earth models. For our first major task, we are performing a comprehensive and methodical evaluation of a set of regional velocity models for Asia based on data misfit and event mislocation metrics. We are currently working with six 3-D regional velocity models of the crust and mantle and are specifically developing our techniques so that they are easily applicable to other models that may become available. In the past year our work on this first task has focused on the accurate conversion of models from their native formats into a single in-house representation and the testing of the numerical tools (such as a set of ray tracing methods) to predict travel times using the models.

In our second task we are developing a new method to evaluate models based on the analysis of their uncertainty. We are currently pursuing a Bayesian approach to this problem in which geostatistical parameters describing velocity uncertainty, together with pick-error variances, are simultaneously fit to the second-order statistics of observed travel-time residuals. To date, we have formulated theoretical solutions within the framework of maximum-likelihood estimation and are seeking practical numerical techniques for computing such solutions.

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